Development of High-Fidelity and Efficient Modeling Capabilities for Enabling Co-Optimization of Fuels and Multi-Mode Engines

Project ID: ace152

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2022 Annual Merit Review

U.S. Department of Energy's (DOE) Vehicle Technologies Office

Stanford University UCONN | UNIVERSITY OF CONNECTICUT Argonne NATIONAL LABORATORY

Overview

Timeline

- Project start: 10/01/2019
- Project end: 3/31/2023
- Percent complete: <75%

Project Partners:

- University of Connecticut: Prof. T. Lu
- Argonne National Lab: Drs. P. Pal, M. Ameen

Budget:

- DOE: $159,953
- Cost-share: $93,786

Barriers

- Co-optimization of fuel and engine
- Extend lean-combustion to intermediate and high-load conditions
- Investigation of new ignition systems
- Improve understanding and modeling of multimode combustion and emissions formation, as well as their interaction with chamber/piston geometry

Relevance

Impact

- Co-optimization of fuels and engines has potential for significant gains in engine performance and efficiency
- Extension of operating condition to high-load range through multi-mode combustion regimes and spark-assisted compression ignition
- Need for accurate and reliable high-fidelity modeling tools to enable successful implementation, control, and optimization of multi-mode combustion regimes, high-energy ignition processes, and wall-heat transfer

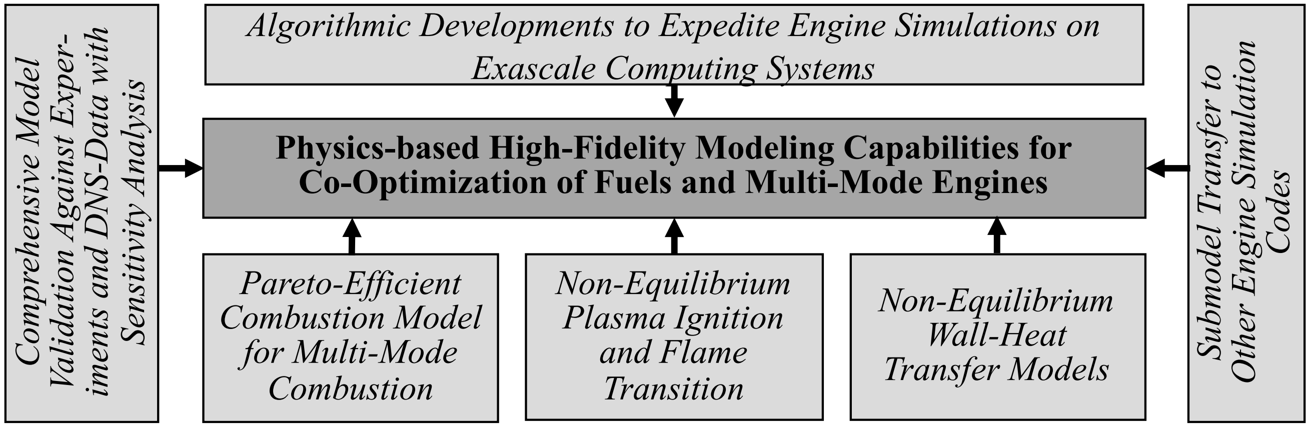
Objectives: Develop improved physical models and numerical algorithms to enable reliable predictions of multi-mode combustion to support EERE's Co-Optima program

- Develop accurate submodels for predicting multi-mode combustion regimes, wall-heat transfer, ignition, and combustion-mode transition
- Develop numerical algorithms and efficient time-integration schemes for exascale computing
- Validate computational submodels against experiments and DNS data

Approach

Develop improved physical models and numerical algorithms for predicting multi-mode combustion

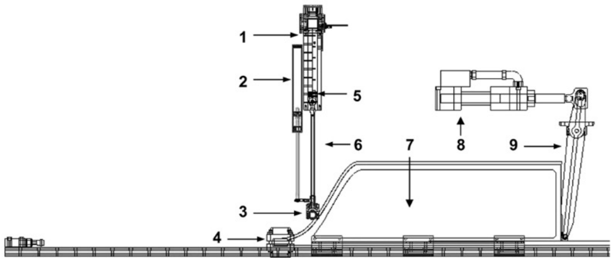
- Task 1 – Fidelity-adaptive combustion-modeling for predicting complex multimode combustion regimes
- Task 2 – Plasma ignition modeling
- Task 3 – Non-equilibrium wall-heat transfer model for prediction of heat-transfer in ICEs
- Task 4 – Multi-mode engine simulations on exascale platform with Nek5000

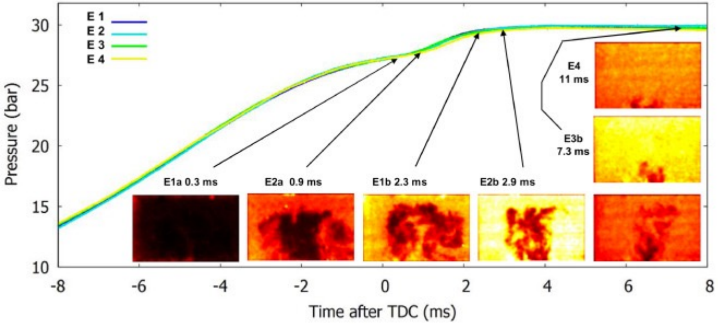


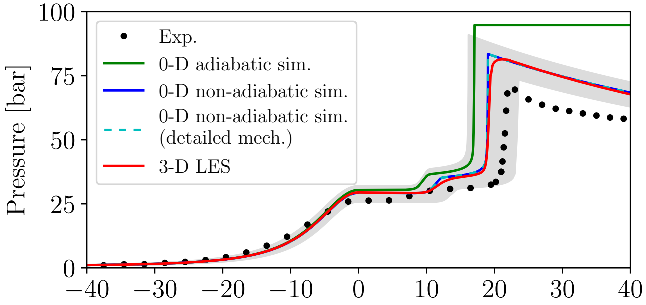
Technical Accomplishments and Progress (Stanford)

Task 1: Multimode combustion modeling

- Goal: examine effects of low-temperature chemistry on ignition delay in rapid compression machines (RCM)
  - LES of RCM configuration by Strozzi et. al.
  - Quarter domain with 0.56 M cells
  - LES with mesh deformation considered with ALE
  - Combustion chemistry: reduced 99-species (+44 QSS species) iso-octane mechanism





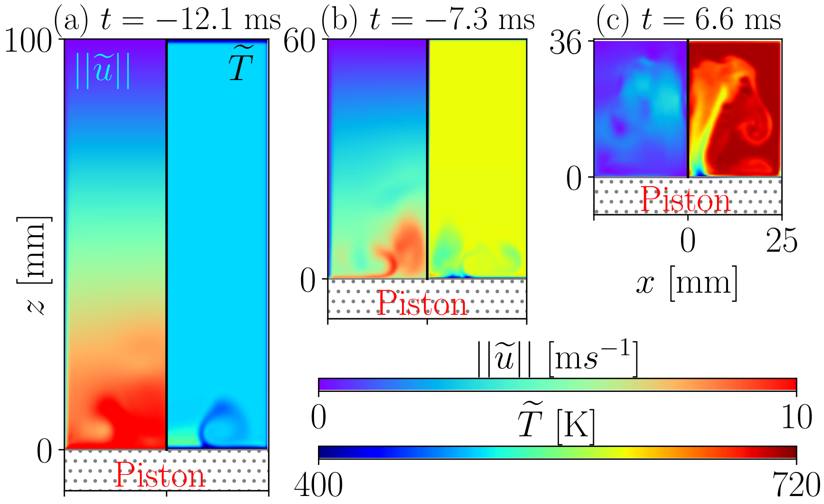


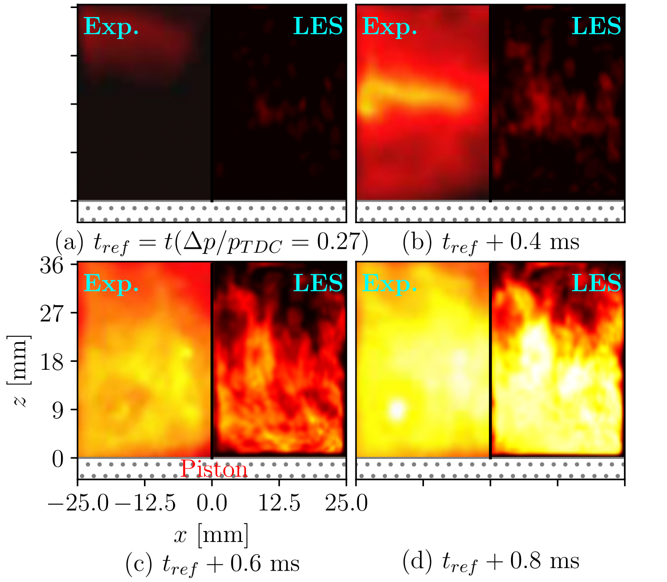
C. Strozzi, A. Claverie, V. Prevost, J. Sotton, M. Bellenoue, *Combust. Flame* (2019).
C. W. Hirt, A. A. Amsden, J. L. Cook, *J. Comput. Phys.* (1974).
C. S. Yoo, Z. Luo, T. Lu, H. Kim, J. H. Chen, *Proc. Combust. Inst.* (2013).
M. Mehl, W. J. Pitz, M. Sj¨oberg, J. E. Dec, *SAE Paper 2009-01-1806* (2009).

Technical Accomplishments and Progress (Stanford)

Task 1: Multimode combustion modeling

- Simulation results
  - Flow field dynamics
  - Comparison with experiments



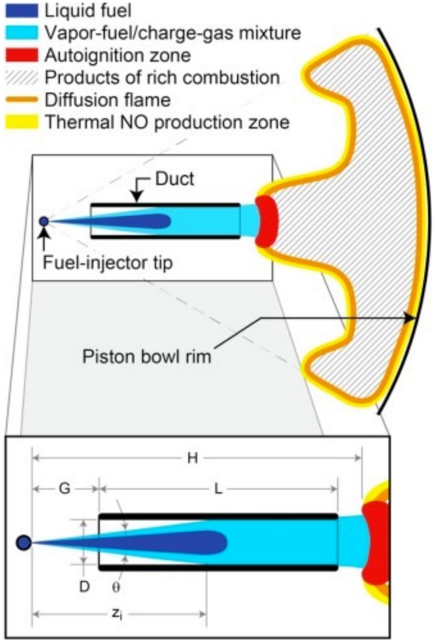


W. T. Chung, N. Ly, and M. Ihme, Accepted for Int. Symp. Combustion, 2022

Technical Accomplishments and Progress (Stanford)

Task 1: Multimode combustion modeling

- Goal: Examine ducted fuel injection (60bar, 1000K)
  - Duct enhances turbulent mixing, lowering equivalence ratios, preventing soot formation
- Computational setup
  - LES of fuel-spray injection with a duct for enhanced fluid mixing and attenuated soot formation
  - Cylindrical domain with 2.2 M cells
  - Diffuse-interface methods for transcritical flows
  - Two-equation soot model
  - Reaction chemistry: 33-species (+21 QSS species) for dodecane

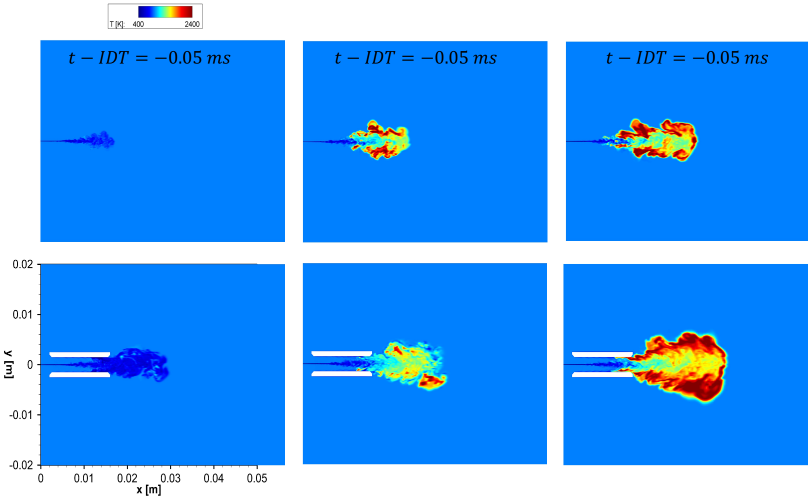


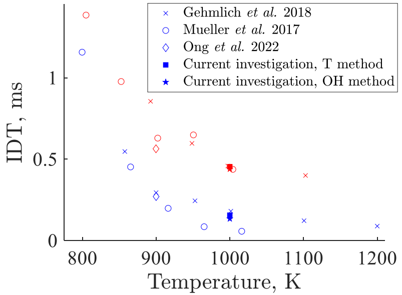
C. J. Mueller, C. W. Nilsen, D. J. Ruth, R. K. Gehmlich, L. M.Pickett, S. A. Skeen, *Appl. Energy* (2017).

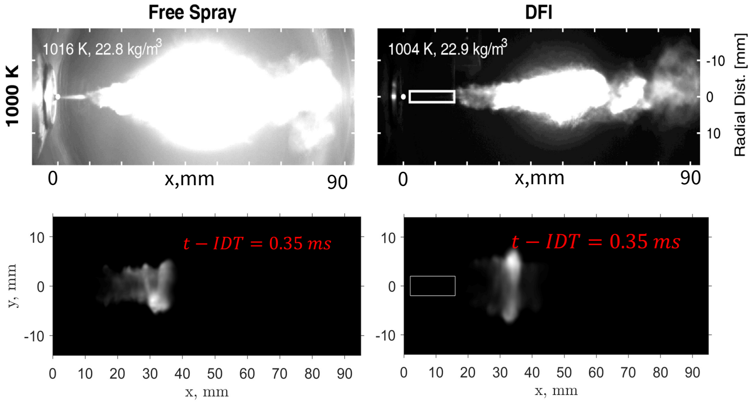
Technical Accomplishments and Progress (Stanford)

Task 1: Multimode combustion modeling

- Results: Comparison with free-jet (Spray A) and DFI-simulation



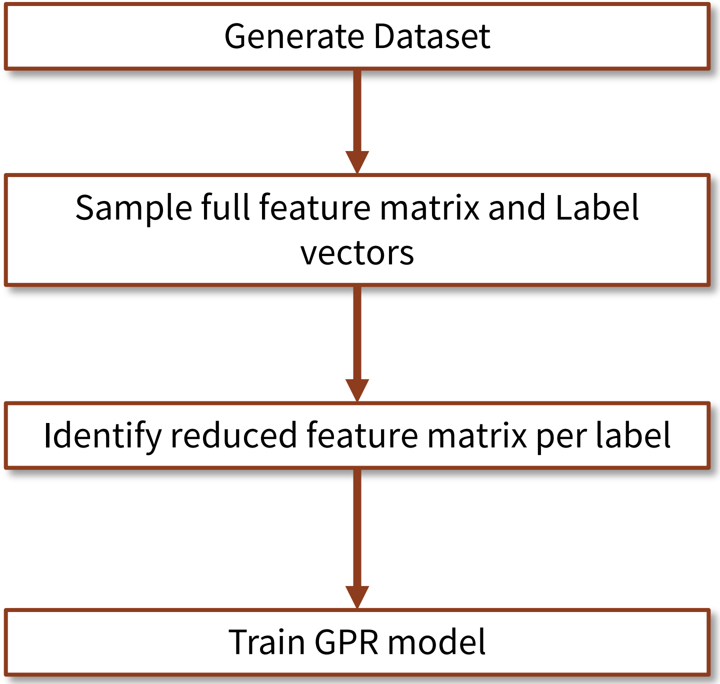




Technical Accomplishments and Progress (UConn)

Task 2: High-energy ignition modeling

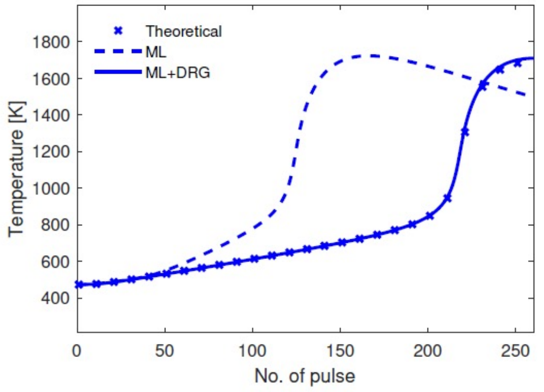
- Motivation:
  - Non-equilibrium plasma chemistry needs to be modeled in multi-dimensional simulations due to its stiffness and strong coupling with electric field
  - Machine learning (ML) based models can reproduce relaxed plasma kinetic effects and avoid resolving non-equilibrium plasma kinetics during engine simulations
- Machine Learning Framework:
  - Generate a dataset of 0D ignition simulations
  - Use directed relation graph (DRG) to reduce the feature matrix for the source terms
  - A ML model for each source term is trained with the reduced feature matrices

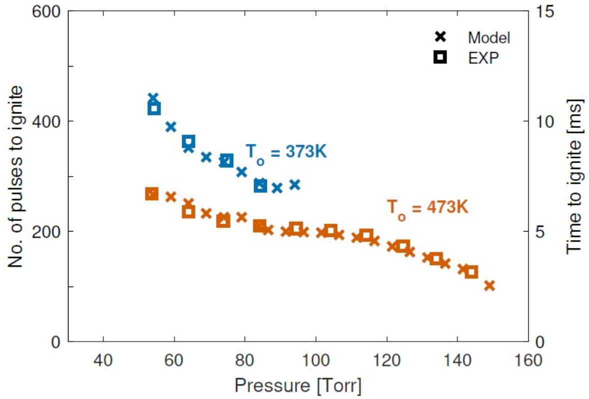


Technical Accomplishments and Progress (UConn)

Task 2: High-energy ignition modeling

- Training data obtained from Boltzmann solver:
  - $\{(x_i, y_i)\ ; i = 1,2, \dots, n\}$ where n is number of sample points
    - x_i : input features $\{\boldsymbol{P\ T\ X_{1:kk}}\}$
    - y_i : targets (source terms) to be predicted $\Delta X_{1:kk} \quad /pulse$
- Network configuration
  - Gaussian process regression (GPR) with an exponential kernel
- Based on the same dataset two ML models were trained:
  1. Based on the full feature matrix
  2. Based on reduced feature matrix
- Ignition delay time accurately predicted with models based on the reduced features





Technical Accomplishments and Progress (ANL)

Task 3: Wall Modeling in Nek5000

- Motivation:
  - With high-order methods, under-resolved turbulent simulations lead to log-law mismatch and oscillations
  - Many finite-volume based wall-models are not well suited for high-order methods
  - High-order methods allow to modify representation of solution
- Enrichment wall model:
  - $\mathrm{u} = u^0 + \psi = \sum_{\mathrm{i}} \phi_i u_i + \psi$
  - When representing the solution, add a physics-based ansatz enrichment function that represents features that are not resolved by the polynomial modes
  - Use the Reichardt law-of-the-wall as the enrichment function in the wall-adjacent elements

$$\psi = u_\tau\left(\frac{1}{0.41}\log(1 + 0.41y^+) + 7.8\left(1 - e^{-\frac{y^+}{11}} - \frac{y^+}{11} e^{-\frac{y^+}{3}}\right)\right)$$

  - Enrichment function captures the mean velocity, while the polynomial terms represent local fluctuations
  - Substituting the enriched solution into the governing equation leads to additional source terms

S.R. Brill, P. Pal, M. Ameen, C. Xu, and M. Ihme, AIAA SciTech Paper 2022-1206 (2022).

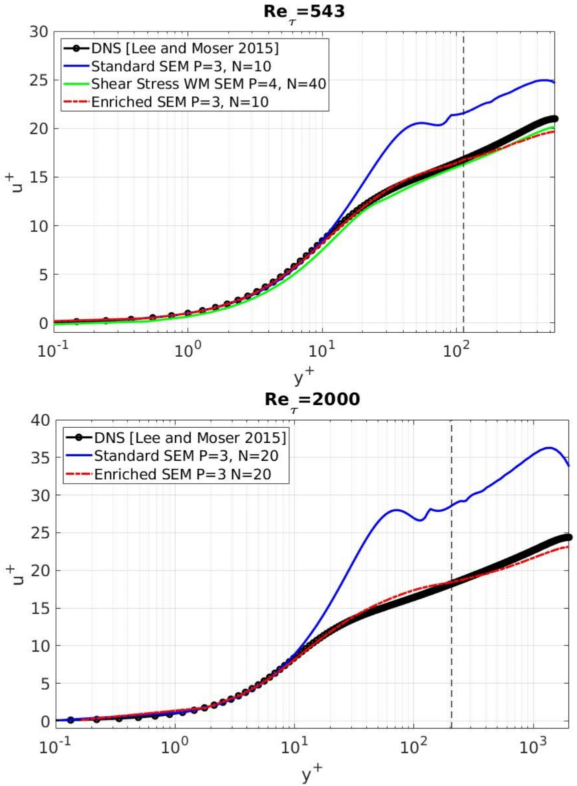
Technical Accomplishments and Progress (ANL)

Task 3: Wall Modeling in Nek5000

- Turbulent Channel Flow
- $Re_\tau = 543, 2000$
- Mesh: N x N x N
- Polynomial Order: P

- Enrichment model performs similar to shear stress wall models with 4x fewer elements

- Stabilizes turbulent flows up to $Re_\tau = 2000$ with a first element of size $y^+ = 200$



S.R. Brill, P. Pal, M. Ameen, C. Xu, and M. Ihme, AIAA SciTech Paper 2022-1206 (2022).

Technical Accomplishments and Progress (ANL)

Task 4: Multi-mode engine simulations with Nek5000

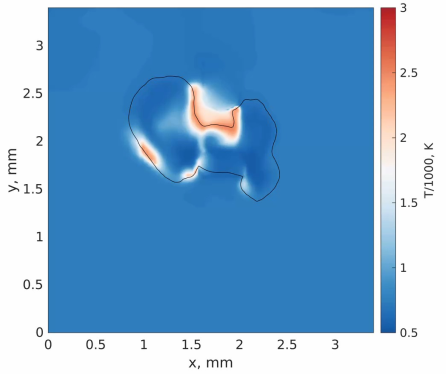
- 2D DNS of initial flame development for a E30 TPRF-E surrogate under partial fuel stratification (PFS)-assisted SACI engine operation

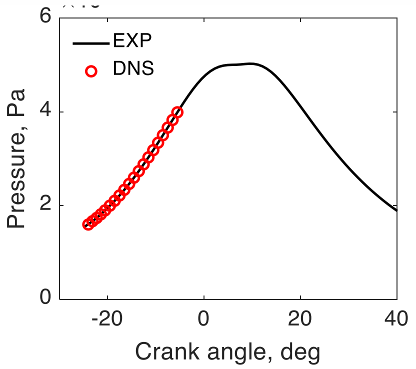
- Realistic initial conditions prescribed from an LES of PFS-assisted lean SACI in Sandia DISI engine

- 90-species reduced TPRF-E chemical kinetic mechanism developed by UConn

- An artificial mass source term added to the continuity equation to ensure that pressure rise in DNS follows exactly the pressure rise in the experiment

DNS – SACI Combustion



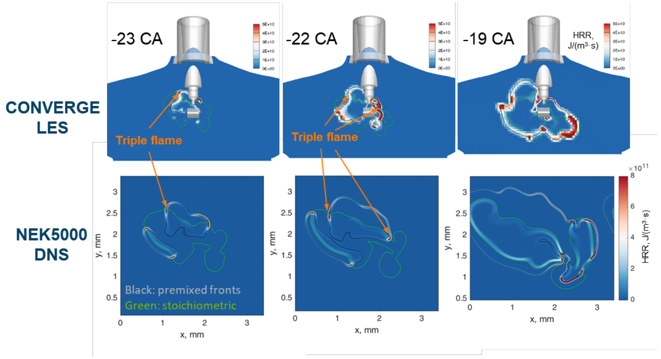


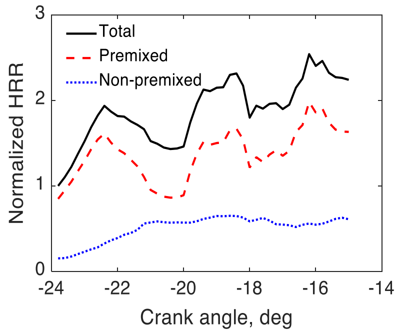
C. Xu, M. Ameen, P. Pal, and S. Som, ASME ICEF2021-67835 (2021).

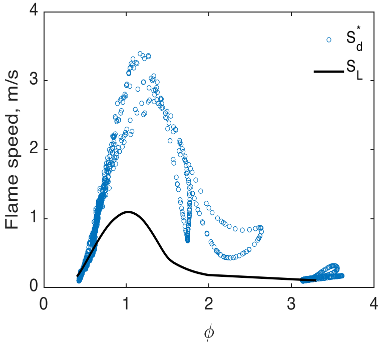
Technical Accomplishments and Progress (ANL)

Task 4: Multi-mode engine simulations with Nek5000

- DNS shows that initial flame development in PFS operation is partially premixed and partially non-premixed, and exhibits triple flame structures
- Similar flame features are captured by both DNS and LES with WSR+G-equation model, indicating the validity of the combustion modeling approach
- Using CEMA-based flame segmentation, locally non-premixed and premixed zones are identified, with premixed flames contributing more dominantly to the total heat release rate (HRR) than the non-premixed mode
- For very lean mixtures, displacement speeds and unstretched laminar flame speeds were identical, while significantly larger values were observed for the displacement speeds under stoichiometric and rich mixtures: **Lewis number effect plays a major role**







C. Xu, M. Ameen, P. Pal, and S. Som, ASME ICEF2021-67835 (2021).

Collaboration and Coordination with Other Institutions

- Ignition modeling
  - Sandia National Labs (Dr. Jackie Chen)
    - DNS analysis
- Nek5000 model development
  - Drs. Saumil Patel, Juan Colmenares (ANL)
  - Prof. Paul Fischer (UIUC)
- Combustion modeling
  - Dr. Camille Strozzi (CNRS): Experimental data for multimode RCM
  - Sandia National Labs: DISI engine experimental data

Proposed Future Research

Task 1: Pareto-efficient combustion model for multi-mode combustion

- PEC-drift term formulation for multimode combustion
- Validation of PEC against multi-mode RCM

Task 2: High-energy ignition model

- High-energy discharge model; Implement plasma equations; Extend model reduction methods to plasma kinetics
- Analyze ignition model against DNS, and validate against Sandia spark calorimeter

Task 3: Non-equilibrium wall-heat transfer model

- Testing enrichment model for wall-bounded turbulent flows with heat transfer
- Formulation of non-equilibrium wall model for variational spectral element method

Task 4: Multi-mode engine simulations with Nek5000

- Algorithmic developments in Nek5000
- Benchmark simulation of TCC-III engine with Nek5000

Summary

Develop improved physical submodels and numerical algorithms to enable accurate and efficient predictions of multi-mode combustion to support EERE's Co-Optima program

- Adaptive LES-combustion model utilizing Pareto-efficient combustion framework for multimode combustion and ignition transition
- Chemical reduction strategies for plasma-ignition
- Non-equilibrium wall model for prediction wall-heat transfer
- Model transition into open-source exascale Nek5000 computing platform

Products and visibility

- W. T. Chung, N. Ly, and M. Ihme, "LES of HCCI combustion of iso-octane/air in a flat-piston rapid compression machine", Int. Symposium Combustion 2022 (accepted).
- J. Guo, W. T. Chung, and M. Ihme, "Computational Analysis of Ducted Fuel Injection at High-Pressure Transcritical Conditions using Large-eddy Simulations", THIESEL 2022 (accepted).
- S.R. Brill, P. Pal, M.M. Ameen, C. Xu, and M. Ihme, "An enrichment wall model for the spectral element method", AIAA SciTech Forum and Exposition, Paper AIAA 2022-1206, 2022.
- P. Pal, M.M. Ameen, and C. Xu, "Near-wall modeling of turbulent flow and heat transfer using a spectral element CFD solver", AIAA SciTech Forum and Exposition, Paper AIAA 2022-1369, 2022.
- C. Xu, M.M. Ameen, P. Pal, and S. Som, "Direct numerical simulation of a reacting hydrogen jet in a turbulent vitiated crossflow using spectral element method", AIAA SciTech Forum and Exposition, Paper AIAA 2022-0823, 2022.
- C. Xu, M. Ameen, P. Pal, and S. Som, "Direct numerical simulation of partial fuel stratification assisted lean premixed combustion for assessment of hybrid G-equation/well-stirred reactor model", ASME Internal Combustion Engine Fall Technical Conference, Paper number ICEF2021-67835, V001T06A005, 2021.
- I. Kabil and T. Lu, "Feature selection for gaussian process regression models of plasma assisted ignition using directed relation graphs", Spring technical meeting of Eastern States Sections of the Combustion Institute, 2022.